The kinetic coefficient of hard-sphere crystal-melt interfaces from molecular-dynamics simulations

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Abstract:

The kinetic coefficient for a crystal melt interface, μ, is the ratio of the interface growth velocity to the undercooling (TM−T), where TM is the melting point. In this work we determine the kinetic coeffiecient for the hard-sphere system by analyzing capillary fluctuations in interface position using molecular dynamics (MD) simulation [Hoyt \emph{et al}, Mat. Sci. Eng. R 41, 121-163 (2003)]. We report the kinetic coefficient for the three interfaces: (100), (110), and (111). Our results for μ100,μ110, and μ111 are 1.15(4) (kB/(mTM))1/2, 0.85(6) (kB/(mTM))1/2, and 0.57(8) (kB/(mTM))1/2, respectively, which gives the relation μ100>μ110>μ111. This ordering is consistent with the recent results of MD simulations for a variety of metals. The anisotropy ratios μ100/μ110, and μ100/μ111 are 1.35(11), and 2.0(3), respectively. We compare our results to those of classical density functional theory (DFT) of [Mikheev and Chernov, J. Cryst. Growth 112, 591-596 (1991)]